# Guido Raos

## List of Publications by Year in descending order

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|---|---|---|---|
| 103 papers | 3,377 citations | 159358 30 h-index | 161609 54 g-index |
| 105 all docs | 105 docs citations | 105 times ranked | 3923 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Theories and simulations of polymer-based nanocomposites: From chain statistics to reinforcement. Progress in Polymer Science, 2008, 33, 683-731. | 11.8 | 256 |
| 2 | Interaction of Water with the Model Ionic Liquid [bmim][BF<sub>4</sub>]: Molecular Dynamics Simulations and Comparison with NMR Data. Journal of Physical Chemistry B, 2008, 112, 7826-7836. | 1.2 | 231 |
| 3 | Halogen Bonding in Fluoroalkylhalides:Â A Quantum Chemical Study of Increasing Fluorine Substitution. Journal of Physical Chemistry A, 2000, 104, 1617-1620. | 1.1 | 198 |
| 4 | The Local Structure of Ionic Liquids: Cationâ€“Cation NOE Interactions and Internuclear Distances in Neat [BMIM][BF4] and [BDMIM][BF4]. Angewandte Chemie - International Edition, 2006, 45, 1123-1126. | 7.2 | 142 |
| 5 | Computational reinvestigation of the bithiophene torsion potential. Chemical Physics Letters, 2003, 379, 364-372. | 1.2 | 121 |
| 6 | Computational Experiments on Filled Rubber Viscoelasticity:Â What Is the Role of Particleâ^'Particle Interactions?. Macromolecules, 2006, 39, 6744-6751. | 2.2 | 104 |
| 7 | Structural Organization and Transport Properties of Novel Pyrrolidinium-Based Ionic Liquids with Perfluoroalkyl Sulfonylimide Anions. Journal of Physical Chemistry B, 2009, 113, 10750-10759. | 1.2 | 102 |
| 8 | Side-Chain Role in Chemically Sensing Conducting Polymer Field-Effect Transistors. Journal of Physical Chemistry B, 2003, 107, 7589-7594. | 1.2 | 101 |
| 9 | Molecular Modeling of Crystalline Alkylthiophene Oligomers and Polymers. Journal of Physical Chemistry B, 2010, 114, 1591-1602. | 1.2 | 87 |
| 10 | Methodological assessment of kinetic Monte Carlo simulations of organic photovoltaic devices: The treatment of electrostatic interactions. Journal of Chemical Physics, 2010, 132, 094705. | 1.2 | 74 |
| 11 | Organicâ^'Organic Epitaxy of Incommensurate Systems:Â Quaterthiophene on Potassium Hydrogen Phthalate Single Crystals. Journal of the American Chemical Society, 2006, 128, 13378-13387. | 6.6 | 71 |
| 12 | Molecular Modeling of Crystalline Oligothiophenes:Â Testing and Development of Improved Force Fields. Journal of Physical Chemistry B, 2004, 108, 18053-18064. | 1.2 | 69 |
| 13 | Blending ionic liquids: how physico-chemical properties change. Physical Chemistry Chemical Physics, 2010, 12, 1784. | 1.3 | 69 |
| 14 | Free Energies of Molecular Crystal Surfaces by Computer Simulation:Â Application to Tetrathiophene. Journal of the American Chemical Society, 2006, 128, 1408-1409. | 6.6 | 63 |
| 15 | Pyrrolidinium-Based Ionic Liquids Doped with Lithium Salts: How Does Li<sup>+</sup> Coordination Affect Its Diffusivity?. Journal of Physical Chemistry B, 2014, 118, 13679-13688. | 1.2 | 63 |
| 16 | Polymer Adhesion: Seeking New Solutions for an Old Problem. Macromolecules, 2021, 54, 10617-10644. | 2.2 | 59 |
| 17 | Chain collapse and phase separation in poorâ€solvent polymer solutions: A unified molecular description. Journal of Chemical Physics, 1996, 104, 1626-1645. | 1.2 | 54 |
| 18 | Ordered Stacking of Regioregular Head-to-Tail Polyalkylthiophenes: Insights from the Crystal Structure of Form Iâ€² Poly(3-n-butylthiophene). Chemistry of Materials, 2009, 21, 78-87. | 3.2 | 50 |

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|---|---|---|---|
| 19 | Nonequilibrium simulations of filled polymer networks: Searching for the origins of reinforcement and nonlinearity. Journal of Chemical Physics, 2011, 134, 054902. | 1.2 | 50 |
| 20 | Pyrazolium- versus Imidazolium-Based Ionic Liquids: Structure, Dynamics and Physicochemical Properties. Journal of Physical Chemistry B, 2013, 117, 668-676. | 1.2 | 49 |
| 21 | Modeling of Molecular Packing and Conformation in Oligofluorenes. Journal of Physical Chemistry B, 2006, 110, 5253-5261. | 1.2 | 48 |
| 22 | Solvent-free phenyl-C61-butyric acid methyl ester (PCBM) from clathrates: insights for organic photovoltaics from crystal structures and molecular dynamics. Chemical Communications, 2013, 49, 4525. | 2.2 | 47 |
| 23 | Interplay of Conformational States and Nonbonded Interactions in Substituted Bithiophenes. Journal of Physical Chemistry A, 2004, 108, 691-698. | 1.1 | 44 |
| 24 | Form II Poly(3-butylthiophene): Crystal Structure and Preferred Orientation in Spherulitic Thin Films. Macromolecules, 2010, 43, 6772-6781. | 2.2 | 43 |
| 25 | Electron transport in crystalline PCBM-like fullerene derivatives: a comparative computational study. Journal of Materials Chemistry C, 2014, 2, 7313-7325. | 2.7 | 41 |
| 26 | Macromolecular clusters in poor-solvent polymer solutions. Journal of Chemical Physics, 1997, 107, 6479-6490. | 1.2 | 39 |
| 27 | Pair populations and effective valencies from ab initio SCF and spin-coupled wave functions. International Journal of Quantum Chemistry, 1996, 57, 501-518. | 1.0 | 36 |
| 28 | Incommensurate Epitaxy of Tetrathiophene on Potassium Hydrogen Phthalate:â€‰ Insights from Molecular Simulation. Crystal Growth and Design, 2006, 6, 1826-1832. | 1.4 | 34 |
| 29 | Application of the Christensen-Lo Model to the Reinforcement of Elastomers by Fractal Fillers. Macromolecular Theory and Simulations, 2003, 12, 17-23. | 0.6 | 33 |
| 30 | Strategies for two-dimensional growth of organic molecular films. Chemical Physics, 2006, 325, 193-206. | 0.9 | 33 |
| 31 | Intramolecular CH/Ï€ interactions in alkylaromatics: Monomer conformations for poly(3â€alkylthiophene) atomistic models. International Journal of Quantum Chemistry, 2013, 113, 2154-2162. | 1.0 | 31 |
| 32 | On the role of different spin bases within spin-coupled theory. Molecular Physics, 1993, 79, 197-216. | 0.8 | 29 |
| 33 | Molecular dynamics simulations of the solvent- and thermal history-dependent structure of the PCBM fullerene derivative. Journal of Materials Chemistry, 2012, 22, 5434. | 6.7 | 29 |
| 34 | The Lowest Singlet and Triplet States of oâ€Benzyne: Spinâ€Coupled Interpretation of the Electronic Structure at CAS SCF Equilibrium Geometries. Israel Journal of Chemistry, 1993, 33, 253-264. | 1.0 | 27 |
| 35 | A Solid State Density Functional Study of Crystalline Thiophene-Based Oligomers and Polymers. Journal of Physical Chemistry B, 2012, 116, 14504-14509. | 1.2 | 27 |
| 36 | Coarseâ€Grained Simulations of Model Polymer Nanofibres. Macromolecular Theory and Simulations, 2011, 20, 305-319. | 0.6 | 26 |

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| 37 | A Cluster of Chains Can Be Smaller Than a Single Chain:Â New Interpretation of Kinetics of Collapse Experiments. Macromolecules, 1996, 29, 8565-8567. | 2.2 | 24 |
| 38 | From Nanoscale to Microscale: Crossover in the Diffusion Dynamics within Two Pyrrolidinium-Based Ionic Liquids. Journal of Physical Chemistry Letters, 2017, 8, 5196-5202. | 2.1 | 23 |
| 39 | Molecular dynamics simulation of rupture in glassy polymer bridges within filler aggregates. Physical Review E, 2012, 86, 041801. | 0.8 | 22 |
| 40 | Improving the efficiency of P3HT:perylene diimide solar cells via bay-substitution with fused aromatic rings. RSC Advances, 2013, 3, 9185. | 1.7 | 22 |
| 41 | An Effective Two-Orbital Quantum Chemical Model for Organic Photovoltaic Materials. Journal of Chemical Theory and Computation, 2014, 10, 364-372. | 2.3 | 21 |
| 42 | Tetrathiophene on Graphite: Molecular Dynamics Simulations. Macromolecular Theory and Simulations, 2004, 13, 497-505. | 0.6 | 20 |
| 43 | Numerical simulation of photocurrent generation in bilayer organic solar cells: Comparison of master equation and kinetic Monte Carlo approaches. Journal of Chemical Physics, 2013, 139, 024706. | 1.2 | 20 |
| 44 | Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. I. Theory and first applications. Chemical Physics, 1994, 186, 233-250. | 0.9 | 19 |
| 45 | Structure of an Associating Polymer Melt in a Narrow Slit by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2005, 109, 18117-18126. | 1.2 | 19 |
| 46 | Conformational Analysis of 2,2â€˜-Bithiophene:Â A1H Liquid Crystal NMR Study Using the13C Satellite Spectra. Journal of Physical Chemistry A, 2005, 109, 9953-9963. | 1.1 | 19 |
| 47 | Role of Desorption in the Growth Process of Molecular Organic Thin Films. Journal of Physical Chemistry B, 2005, 109, 7859-7864. | 1.2 | 19 |
| 48 | Atomistic Simulation of Phase Transitions and Charge Mobility for the Organic Semiconductor Ph-BTBT-C10. Chemistry of Materials, 2019, 31, 7092-7103. | 3.2 | 19 |
| 49 | Viscoelasticity of Short Polymer Liquids from Atomistic Simulations. Journal of the Electrochemical Society, 2019, 166, B3246-B3256. | 1.3 | 19 |
| 50 | Spin-Coupled Study of the Electronic Structure of Polyenyl Radicals C3H5-C9H11. Journal of the American Chemical Society, 1994, 116, 2075-2084. | 6.6 | 18 |
| 51 | Polymer association in poor solvents: from monomolecular micelles to clusters of chains and phase separation. Macromolecular Theory and Simulations, 1999, 8, 65-84. | 0.6 | 18 |
| 52 | Mesoscopic bead-and-spring model of hard spherical particles in a rubber matrix. I. Hydrodynamic reinforcement. Journal of Chemical Physics, 2000, 113, 7554-7563. | 1.2 | 18 |
| 53 | The collapse of chains with different architectures. Journal of Chemical Physics, 1994, 100, 7804-7813. | 1.2 | 17 |
| 54 | Structure of Model Telechelic Polymer Melts by Computer Simulation. Journal of Macromolecular Science - Physics, 2005, 44, 855-871. | 0.4 | 17 |

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| 55 | Impact of Interaction Strength and Surface Heterogeneity on the Dynamics of Adsorbed Polymers. ACS Macro Letters, 2014, 3, 721-726. | 2.3 | 17 |
| 56 | Spin-Coupled Valence Bond Study of the Reaction between Benzene and a Methyl Cation. Journal of Physical Chemistry A, 1997, 101, 2886-2892. | 1.1 | 16 |
| 57 | Effects of chemically heterogeneous nanoparticles on polymer dynamics: insights from molecular dynamics simulations. Soft Matter, 2018, 14, 1219-1226. | 1.2 | 16 |
| 58 | Glassy dynamics of a polymer monolayer on a heterogeneous disordered substrate. Soft Matter, 2015, 11, 8083-8091. | 1.2 | 15 |
| 59 | Influence of wall heterogeneity on nanoscopically confined polymers. Physical Chemistry Chemical Physics, 2019, 21, 772-779. | 1.3 | 15 |
| 60 | Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. Journal of Physical Chemistry B, 1997, 101, 6688-6691. | 1.2 | 14 |
| 61 | Hydrophobic aggregation and collective absorption of dioxin into lipid membranes: insights from atomistic simulations. Physical Chemistry Chemical Physics, 2015, 17, 2344-2348. | 1.3 | 14 |
| 62 | Molecular dynamics simulation of metallic impurity diffusion in liquid lead-bismuth eutectic (LBE). Journal of Nuclear Materials, 2018, 501, 253-260. | 1.3 | 14 |
| 63 | Spin correlation in Ï€-electron systems from spin-coupled wavefunctions. II. Further applications. Chemical Physics, 1994, 186, 251-273. | 0.9 | 13 |
| 64 | Chain Interactions in Poor-Solvent Polymer Solutions:â€‰ Equilibrium and Nonequilibrium Aspects. Macromolecules, 1996, 29, 6663-6670. | 2.2 | 13 |
| 65 | Degrees of Chirality in Helical Structures. Macromolecular Theory and Simulations, 2002, 11, 739-750. | 0.6 | 13 |
| 66 | Functionalized Oligothiophenes for Optoelectronic Applications:â€‰ 3â€˜,4â€˜,3â€˜â€‰â€˜â€˜,4â€˜â€‰â€˜â€˜-Tetra [(methoxycarbonyl)methyl]-2,2â€˜:5â€˜,2â€˜â€‰â€˜:5â€˜â€‰â€˜,2â€˜â€‰â€˜â€˜:5â€˜â€‰â€˜â€˜,2â€˜â€‰â€˜â€˜â€‰â€‰quinquithi Materials, 2005, 17, 242-249. | 3.2 | 13 |
| 67 | Organic Peracids: A Structural Puzzle for <sup>17</sup>O NMR and Ab Initio Chemical Shift Calculations. Journal of Physical Chemistry A, 2012, 116, 1814-1819. | 1.1 | 13 |
| 68 | Coarse-grained kinetic modelling of bilayer heterojunction organic solar cells. Organic Electronics, 2012, 13, 750-761. | 1.4 | 13 |
| 69 | Evidence of superdiffusive nanoscale motion in anionic polymeric hydrogels: Analysis of PGSE- NMR data and comparison with drug release properties. Journal of Controlled Release, 2019, 305, 110-119. | 4.8 | 13 |
| 70 | A Coarse-Grained Force Field for Silicaâ€“Polybutadiene Interfaces and Nanocomposites. Polymers, 2020, 12, 1484. | 2.0 | 12 |
| 71 | Aromatic electrophilic substitution. A modern valence bond study. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4011. | 1.7 | 11 |
| 72 | Origin of Charge Separation at Organic Photovoltaic Heterojunctions: A Mesoscale Quantum Mechanical View. Journal of Physical Chemistry C, 2017, 121, 16693-16701. | 1.5 | 10 |

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| 73 | All-Atom Model of Atactic 2-Vinyl Pyridine Polymer: Structural Properties Investigation by Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2019, 166, B3309-B3315. | 1.3 | 10 |
| 74 | Rigid filler particles in a rubber matrix: effective force constants by multipolar expansion. Computational and Theoretical Polymer Science, 2000, 10, 149-157. | 1.1 | 9 |
| 75 | Materials for organic photovoltaics: insights from detailed structural models and molecular simulations. EPJ Web of Conferences, 2012, 33, 02002. | 0.1 | 9 |
| 76 | Pulling Polymers on Energetically Disordered Surfaces: Molecular Dynamics Tests of Linear and Nonâ€linear Response. Macromolecular Theory and Simulations, 2013, 22, 225-237. | 0.6 | 9 |
| 77 | Fracture in Silica/Butadiene Rubber: A Molecular Dynamics View of Designâ€“Property Relationships. ACS Polymers Au, 0, , . | 1.7 | 9 |
| 78 | Sliding friction between polymer surfaces: A molecular interpretation. Journal of Chemical Physics, 2006, 124, 144713. | 1.2 | 8 |
| 79 | Equilibrium Dynamics of an Associating Polymer Melt in Narrow Slits by Computer Simulation. Journal of Physical Chemistry B, 2007, 111, 4141-4149. | 1.2 | 8 |
| 80 | Computational 17O-NMRspectroscopy of organic acids and peracids: comparison of solvation models. Physical Chemistry Chemical Physics, 2013, 15, 1130-1140. | 1.3 | 8 |
| 81 | The effect of donor content on the efficiency of P3HT:PCBM bilayers: optical and photocurrent spectral data analyses. Physical Chemistry Chemical Physics, 2015, 17, 2447-2456. | 1.3 | 8 |
| 82 | Molecular Dynamics Simulation on Physical Properties of Liquid Lead, Bismuth and Lead-bismuth Eutectic (LBE). Procedia Engineering, 2016, 157, 214-221. | 1.2 | 8 |
| 83 | Atomistic modelling of entropy driven phase transitions between different crystal modifications in polymers: the case of poly(3-alkylthiophenes). Physical Chemistry Chemical Physics, 2018, 20, 28984-28989. | 1.3 | 8 |
| 84 | Magnetic Resonance Imaging and Molecular Dynamics Characterization of Ionic Liquid in Poly(ethylene oxide)-Based Polymer Electrolytes. ACS Applied Materials & Interfaces, 2020, 12, 23800-23811. | 4.0 | 8 |
| 85 | Catalytic chemistry of furan and thiophene. Ab initio calculations, using the spin-coupled valence bond method, of the interaction of furan and thiophene with a positively charged centre. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 749. | 1.7 | 7 |
| 86 | Stereochemically pure Î±-trifluoromethyl-malic hydroxamates: synthesis and evaluation as inhibitors of matrix metalloproteinases. Tetrahedron, 2006, 62, 10171-10181. | 1.0 | 7 |
| 87 | 17O NMR. Annual Reports on NMR Spectroscopy, 2015, 85, 143-193. | 0.7 | 7 |
| 88 | From dioxin to dioxin congeners: understanding the differences in hydrophobic aggregation in water and absorption into lipid membranes by means of atomistic simulations. Physical Chemistry Chemical Physics, 2016, 18, 17731-17739. | 1.3 | 7 |
| 89 | Surface Reconstructions in Organic Crystals: Simulations of the Effect of Temperature and Defectivity on Bulk and (001) Surfaces of 2,2â€²:6â€²,2â€³-Ternaphthalene. Crystal Growth and Design, 2016, 16, 412-422. | 1.4 | 7 |
| 90 | Towards realistic simulations of polymer networks: tuning vulcanisation and mechanical properties. Physical Chemistry Chemical Physics, 2021, 23, 3496-3510. | 1.3 | 7 |

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| 91 | Rigid particles in an elastic polymer network: An electrical-analog approach. Journal of Chemical Physics, 1998, 109, 3285-3292. | 1.2 | 6 |
| 92 | Rotational barriers of amides and polyisocyanates: A spin-coupled study. International Journal of Quantum Chemistry, 1999, 74, 249-258. | 1.0 | 6 |
| 93 | Confined polymer networks: The harmonic approach. Journal of Chemical Physics, 2002, 116, 3109-3118. | 1.2 | 6 |
| 94 | Polymer-mediated adhesion: A statistical approach. Journal of Chemical Physics, 2003, 119, 9295-9307. | 1.2 | 6 |
| 95 | Association and Diffusion of Li<sup>+</sup> in Carboxymethylcellulose Solutions for Environmentally Friendly Liâ€ion Batteries. ChemSusChem, 2016, 9, 1804-1813. | 3.6 | 6 |
| 96 | Tunable interaction potentials and morphology of polymerâ€“nanoparticle blends. Journal of Chemical Physics, 2020, 152, 174902. | 1.2 | 5 |
| 97 | Quo Vadis, Macromolecular Science? Reflections by the IUPAC Polymer Division on the Occasion of the Staudinger Centenary. Israel Journal of Chemistry, 2020, 60, 9-19. | 1.0 | 5 |
| 98 | Identification of viable TCDD access pathways to human AhR PAS-B ligand binding domain. Journal of Molecular Graphics and Modelling, 2021, 105, 107886. | 1.3 | 5 |
| 99 | Polymer-Mediated Adhesion: Nanoscale Surface Morphology and Failure Mechanisms. Macromolecules, 2021, 54, 195-202. | 2.2 | 4 |
| 100 | Substituent effects on the second-order hyperpolarisability of cyanine cations. Computational and Theoretical Chemistry, 2002, 589-590, 439-445. | 1.5 | 3 |
| 101 | Rubber elasticity: A contactâ€probability model with harmonic entanglement constraints. Journal of Chemical Physics, 1996, 105, 8352-8361. | 1.2 | 2 |
| 102 | Polymer Chains and Networks in Narrow Slits. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2005, , 249-268. | 0.1 | 0 |
| 103 | Viscoelasticity of Short Polymer Melts from Atomistic Simulations. ECS Meeting Abstracts, 2018, , . | 0.0 | 0 |